L5 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:523321 CAPLUS Full-text

DN 141:225474

TI Synthesis of C8-linked pyrrolo[2,1-c][1,4]benzodiazepine-acridone/acridine hybrids as potential DNA-binding agents

AU Kamal, Ahmed; Srinivas, O.; Ramulu, P.; Ramesh, G.; Kumar, P. Praveen

CS Division of Organic Chemistry, Indian Institute of Chemical Technology, Hyderabad, 500007, India

SO Bioorganic & Medicinal Chemistry Letters (2004), 14(15), 4107-4111 CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier Science B.V.

DT Journal

LA English

OS CASREACT 141:225474

GΙ

AB Pyrrolobenzodiazepine hybrids linked to acridone/acridine ring systems at C8-position have been designed and prepared These compds. exhibit significant DNA-binding affinity, and a representative compound (I, n = 2) shows promising in vitro anticancer activity.

IT 745014-20-4P 745014-21-5P 745014-22-6P

745014-23-7P
PL. PAC (Pharmagological activity), SDN (Synthotic

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis of C8-linked pyrrolo[2,1-c][1,4]benzodiazepine-acridone/acridine hybrids as potential DNA-binding agents and antitumor agents)

RN 745014-20-4 CAPLUS

CN 4-Acridinecarboxamide, 9,10-dihydro-9-oxo-N-[3-[[(11aS)-2,3,5,11a-tetrahydro-7-methoxy-5-oxo-1H-pyrrolo[2,1-c][1,4]benzodiazepin-8-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 745014-21-5 CAPLUS

CN 4-Acridinecarboxamide, N-[3-[[(11aS)-2,3,5,11a-tetrahydro-7-methoxy-5-oxo-1H-pyrrolo[2,1-c][1,4]benzodiazepin-8-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 745014-22-6 CAPLUS

CN 4-Acridinecarboxamide, 9,10-dihydro-9-oxo-N-[2-[[(11aS)-2,3,5,11a-tetrahydro-7-methoxy-5-oxo-1H-pyrrolo[2,1-c][1,4]benzodiazepin-8-yl]oxy]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 745014-23-7 CAPLUS

CN 4-Acridinecarboxamide, N-[2-[[(11aS)-2,3,5,11a-tetrahydro-7-methoxy-5-oxo-1H-pyrrolo[2,1-c][1,4]benzodiazepin-8-yl]oxy]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Chemical Name (CN): 9-oxo-9,10-dihydro-acridine-4-carboxylic

> acid <3-(7-methoxy-5-oxo-2,3,5,11atetrahydro-1H-benzo<e>pyrrolo<1,2a><1,4>diazepin-8-yloxy)-propyl>-amide

Autonom Name (AUN): 9-oxo-9,10-dihydro-acridine-4-carboxylic

> acid <3-(7-methoxy-5-oxo-2,3,5,11atetrahydro-1H-benzo<e>pyrrolo<1,2a><1,4>diazepin-8-yloxy)-propyl>-amide

Molec. Formula (MF): C30 H28 N4 O5

Molecular Weight (MW): 524.58

Lawson Number (LN): 29107, 27041, 3131, 289

File Segment (FS): Stereo compound Compound Type (CTYPE): heterocyclic

Constitution ID (CONSID): 8276362 Tautomer ID (TAUTID): 9204410 Entry Date (DED): 2005/01/21 Update Date (DUPD): 2005/01/21

Reference(s):

1. Kamal, Ahmed; Srinivas, O.; Ramulu, P.; Ramesh, G.; Kumar, P. Praveen, Bioorg. Med. Chem. Lett., CODEN: BMCLE8, 14(15), <2004>, 4107 - 4112; BABS-6462175

Chemical Name (CN): 9-oxo-9,10-dihydro-acridine-4-carboxylic

acid <2-(7-methoxy-5-oxo-2,3,5,11a-tetrahydro-1H-benzo<e>pyrrolo<1,2-a><1,4>diazepin-8-yloxy)-ethyl>-amide

Autonom Name (AUN): 9-oxo-9,10-dihydro-acridine-4-carboxylic acid <2-(7-methoxy-5-oxo-2,3,5,11a-

tetrahydro-1H-benzo<e>pyrrolo<1,2a><1,4>diazepin-8-yloxy) -ethyl>-amide

Molec. Formula (MF): C29 H26 N4 O5

Molecular Weight (MW): 510.55

Lawson Number (LN): 29107, 27041, 3122, 289

File Segment (FS): Stereo compound Compound Type (CTYPE): heterocyclic

 Constitution ID (CONSID):
 8275088

 Tautomer ID (TAUTID):
 9203427

 Entry Date (DED):
 2005/01/21

 Update Date (DUPD):
 2005/01/21

Reference(s):

 Kamal, Ahmed; Srinivas, O.; Ramulu, P.; Ramesh, G.; Kumar, P. Praveen, Bioorg. Med. Chem. Lett., CODEN: BMCLE8, 14(15), <2004>, 4107 - 4112; BABS-6462175

Chemical Name (CN): acridine-4-carboxylic acid

<3-(7-methoxy-5-oxo-2,3,5,11a-tetrahydro-1H-benzo<e>pyrrolo<1,2-a><1,4>diazepin-8-

yloxy) -propyl>-amide

Autonom Name (AUN): acridine-4-carboxylic acid

<3-(7-methoxy-5-oxo-2,3,5,11a-tetrahydro-1H-benzo<e>pyrrolo<1,2-a><1,4>diazepin-8-

yloxy) -propyl>-amide

Molec. Formula (MF): C30 H28 N4 O4

Molecular Weight (MW): 508.58

Lawson Number (LN): 29107, 26432, 3131, 289

File Segment (FS): Stereo compound Compound Type (CTYPE): heterocyclic

 Constitution ID (CONSID):
 8274346

 Tautomer ID (TAUTID):
 9199876

 Entry Date (DED):
 2005/01/21

 Update Date (DUPD):
 2005/01/21

Reference(s):

 Kamal, Ahmed; Srinivas, O.; Ramulu, P.; Ramesh, G.; Kumar, P. Praveen, Bioorg. Med. Chem. Lett., CODEN: BMCLE8, 14(15), <2004>, 4107 - 4112; BABS-6462175

Chemical Name (CN): acridine-4-carboxylic acid

<2-(7-methoxy-5-oxo-2,3,5,11a-tetrahydro-1H-benzo<e>pyrrolo<1,2-a><1,4>diazepin-8-

yloxy) -ethyl>-amide

Autonom Name (AUN): acridine-4-carboxylic acid

<2-(7-methoxy-5-oxo-2,3,5,11a-tetrahydro-1H-benzo<e>pyrrolo<1,2-a><1,4>diazepin-8-

yloxy) -ethyl>-amide

Molec. Formula (MF): C29 H26 N4 O4

Molecular Weight (MW): 494.55

Lawson Number (LN): 29107, 26432, 3122, 289

File Segment (FS): Stereo compound Compound Type (CTYPE): heterocyclic

 Constitution ID (CONSID):
 8272807

 Tautomer ID (TAUTID):
 9198665

 Entry Date (DED):
 2005/01/21

 Update Date (DUPD):
 2005/01/21

Reference(s):

 Kamal, Ahmed; Srinivas, O.; Ramulu, P.; Ramesh, G.; Kumar, P. Praveen, Bioorg. Med. Chem. Lett., CODEN: BMCLE8, 14(15), <2004>, 4107 - 4112; BABS-6462175 => d 12; d his; log y L2 HAS NO ANSWERS L1 STR

Structure attributes must be viewed using STN Express query preparation. L2 QUE ABB=ON PLU=ON L1

(FILE 'HOME' ENTERED AT 16:55:59 ON 25 MAY 2005)

FILE 'REGISTRY' ENTERED AT 16:56:15 ON 25 MAY 2005

L1 STRUCTURE UPLOADED

L2 QUE L1

L3 0 S L2

L4 4 S L2 FUL

FILE 'CAPLUS' ENTERED AT 16:56:45 ON 25 MAY 2005

L5 1 S L4

FILE 'BEILSTEIN' ENTERED AT 16:57:09 ON 25 MAY 2005

L6 1 S L2

L7 4 S L2 FUL

L8 4 S L7 NOT L4

L9 4 S L7 NOT L5

FILE 'MARPAT' ENTERED AT 16:58:00 ON 25 MAY 2005

L10 0 S L2

L11 0 S L2 FUL

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